NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM
Technical Program Review
March 18-19, 2015

IM #789853

Analytical Methods Update

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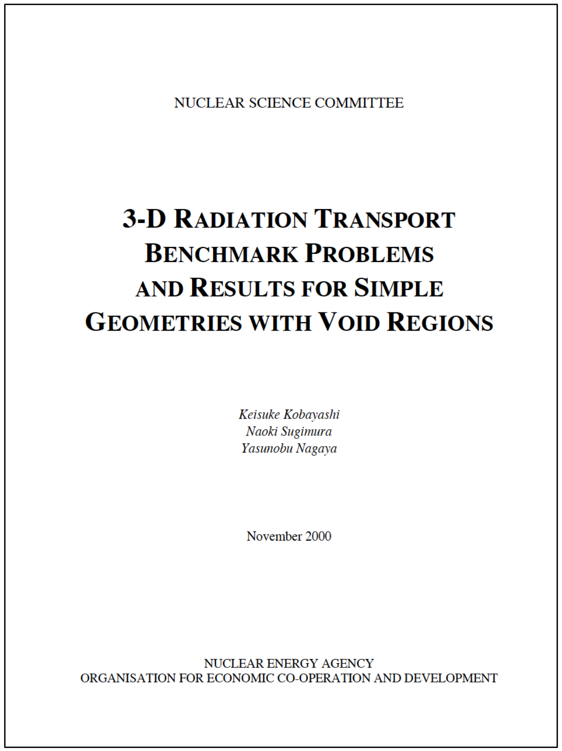
Outline

- Analytic benchmarks
- Alpha particle transport
- Deuteron transport
- Advance (with BNL)
- SQA

COG11.1 will be provided to RSICC in advance of ICNC

Analytic benchmarks completed in FY-2014

Kobayahsi



NUCLEAR SCIENCE COMMITTEE

3-D RADIATION TRANSPORT BENCHMARK PROBLEMS AND RESULTS FOR SIMPLE GEOMETRIES WITH VOID REGIONS

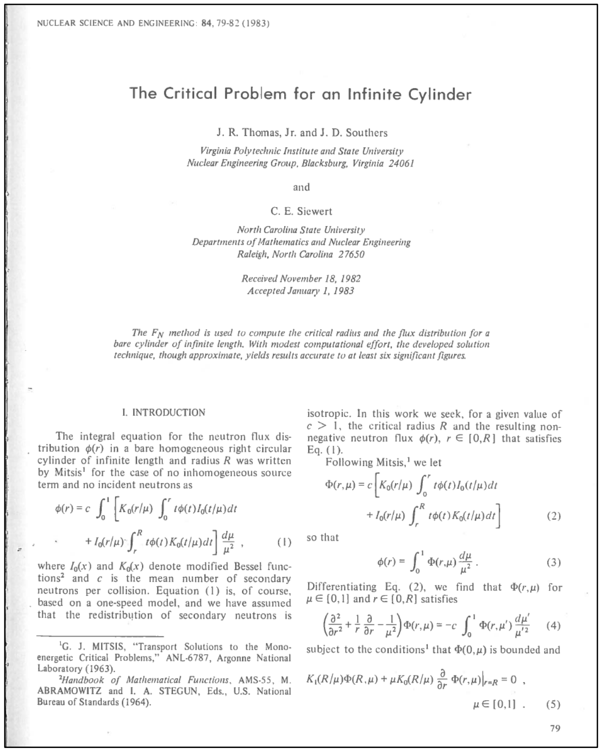
Keisuke Kobayashi
Naoki Sugimura
Yasunobu Nagaya

November 2000

NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

NSC-DOC2000-4 (2000)

Cylinder



NUCLEAR SCIENCE AND ENGINEERING: **84**, 79-82 (1983)

The Critical Problem for an Infinite Cylinder

J. R. Thomas, Jr. and J. D. Southers
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and

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Received November 18, 1982
Accepted January 1, 1983

The F_N method is used to compute the critical radius and the flux distribution for a bare cylinder of infinite length. With modest computational effort, the developed solution technique, though approximate, yields results accurate to at least six significant figures.

I. INTRODUCTION

The integral equation for the neutron flux distribution $\phi(r)$ in a bare homogeneous right circular cylinder of infinite length and radius R was written by Mitsis[1] for the case of no inhomogeneous source term and no incident neutrons as

$$\phi(r) = c \int_0^1 \left[K_0(r/\mu) \int_0^r t\phi(t) I_0(t/\mu)dt + I_0(r/\mu) \int_r^R t\phi(t) K_0(t/\mu)dt\right] \frac{d\mu}{\mu^2} , \quad (1)$$

where $I_0(x)$ and $K_0(x)$ denote modified Bessel functions[2] and c is the mean number of secondary neutrons per collision. Equation (1) is, of course, based on a one-speed model, and we have assumed that the redistribution of secondary neutrons is isotropic. In this work we seek, for a given value of $c > 1$, the critical radius R and the resulting non-negative neutron flux $\phi(r)$, $r \in [0,R]$ that satisfies Eq. (1).

Following Mitsis,[1] we let

$$\Phi(r,\mu) = c\left[K_0(r/\mu) \int_0^r t\phi(t) I_0(t/\mu)dt + I_0(r/\mu) \int_r^R t\phi(t) K_0(t/\mu)dt\right] \quad (2)$$

so that

$$\phi(r) = \int_0^1 \Phi(r,\mu) \frac{d\mu}{\mu^2} . \quad (3)$$

Differentiating Eq. (2), we find that $\Phi(r,\mu)$ for $\mu \in [0,1]$ and $r \in [0,R]$ satisfies

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{1}{\mu^2}\right)\Phi(r,\mu) = -c \int_0^1 \Phi(r,\mu') \frac{d\mu'}{\mu'^2} \quad (4)$$

subject to the conditions[1] that $\Phi(0,\mu)$ is bounded and

$$K_1(R/\mu)\Phi(R,\mu) + \mu K_0(R/\mu) \frac{\partial}{\partial r} \Phi(r,\mu)\Big|_{r=R} = 0 , \quad \mu \in [0,1] . \quad (5)$$

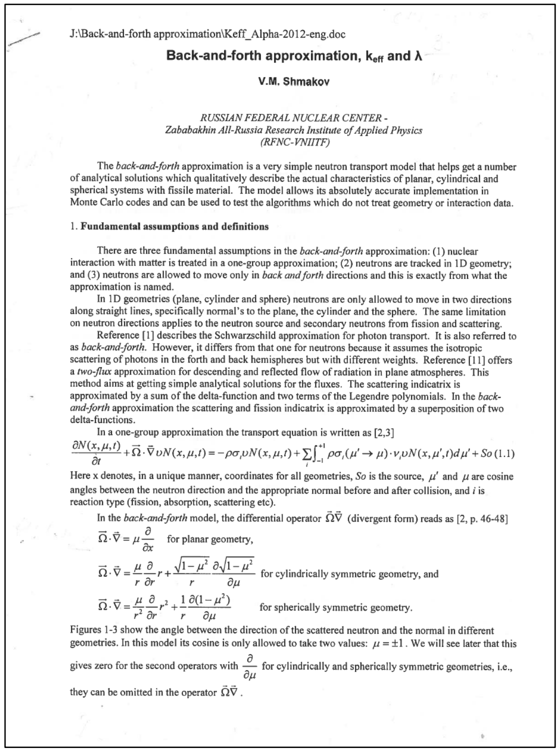
[1]G. J. MITSIS, "Transport Solutions to the Monoenergetic Critical Problems," ANL-6787, Argonne National Laboratory (1963).

[2]*Handbook of Mathematical Functions*, AMS-55, M. ABRAMOWITZ and I. A. STEGUN, Eds., U.S. National Bureau of Standards (1964).

79

NSE **84** 79-82 (1983)

Shmakov



J:\Back-and-forth approximation\Keff_Alpha-2012-eng.doc

Back-and-forth approximation, k_{eff} and λ

V.M. Shmakov

RUSSIAN FEDERAL NUCLEAR CENTER -
Zababakhin All-Russia Research Institute of Applied Physics
(RFNC-VNIITF)

The *back-and-forth* approximation is a very simple neutron transport model that helps get a number of analytical solutions which qualitatively describe the actual characteristics of planar, cylindrical and spherical systems with fissile material. The model allows its absolutely accurate implementation in Monte Carlo codes and can be used to test the algorithms which do not treat geometry or interaction data.

1. **Fundamental assumptions and definitions**

There are three fundamental assumptions in the *back-and-forth* approximation: (1) nuclear interaction with matter is treated in a one-group approximation; (2) neutrons are tracked in 1D geometry; and (3) neutrons are allowed to move only in *back and forth* directions and this is exactly from what the approximation is named.

In 1D geometries (plane, cylinder and sphere) neutrons are only allowed to move in two directions along straight lines, specifically normal's to the plane, the cylinder and the sphere. The same limitation on neutron directions applies to the neutron source and secondary neutrons from fission and scattering.

Reference [1] describes the Schwarzschild approximation for photon transport. It is also referred to as *back-and-forth*. However, it differs from that one for neutrons because it assumes the isotropic scattering of photons in the forth and back hemispheres but with different weights. Reference [11] offers a *two-flux* approximation for descending and reflected flow of radiation in plane atmospheres. This method aims at getting simple analytical solutions for the fluxes. The scattering indicatrix is approximated by a sum of the delta-function and two terms of the Legendre polynomials. In the *back-and-forth* approximation the scattering and fission indicatrix is approximated by a superposition of two delta-functions.

In a one-group approximation the transport equation is written as [2,3]

$$\frac{\partial N(x,\mu,t)}{\partial t} + \vec{\Omega}\cdot\vec{\nabla}\upsilon N(x,\mu,t) = -\rho\sigma_t\upsilon N(x,\mu,t) + \sum_i \int_{-1}^{+1} \rho\sigma_i(\mu' \to \mu)\cdot\nu_i\upsilon N(x,\mu',t)d\mu' + So \quad (1.1)$$

Here x denotes, in a unique manner, coordinates for all geometries, *So* is the source, μ' and μ are cosine angles between the neutron direction and the appropriate normal before and after collision, and i is reaction type (fission, absorption, scattering etc).

In the *back-and-forth* model, the differential operator $\vec{\Omega}\vec{\nabla}$ (divergent form) reads as [2, p. 46-48]

$\vec{\Omega}\cdot\vec{\nabla} = \mu\frac{\partial}{\partial x}$ for planar geometry,

$\vec{\Omega}\cdot\vec{\nabla} = \frac{\mu}{r}\frac{\partial}{\partial r}r + \frac{\sqrt{1-\mu^2}}{r}\frac{\partial\sqrt{1-\mu^2}}{\partial\mu}$ for cylindrically symmetric geometry, and

$\vec{\Omega}\cdot\vec{\nabla} = \frac{\mu}{r^2}\frac{\partial}{\partial r}r^2 + \frac{1}{r}\frac{\partial(1-\mu^2)}{\partial\mu}$ for spherically symmetric geometry.

Figures 1-3 show the angle between the direction of the scattered neutron and the normal in different geometries. In this model its cosine is only allowed to take two values: $\mu = \pm 1$. We will see later that this gives zero for the second operators with $\frac{\partial}{\partial\mu}$ for cylindrically and spherically symmetric geometries, i.e., they can be omitted in the operator $\vec{\Omega}\vec{\nabla}$.

Unpublished manuscript (2012)

COG results published by Ed Lent as LLNL-TR-648225, Three Analytic Benchmarks in COG, and presented at the NCSP TPR at LANL. COG results were generally excellent.

Analytic benchmarks in progress

Data Bank

ISBN 978-92-64-99056-2
NEA/DB/DOC(2008)1

Analytical Benchmarks
for Nuclear Engineering Applications

Case Studies in Neutron Transport Theory

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Department of Aerospace and Mechanical Engineering
University of Arizona

with Forewords by

Paul F. Zweifel
Richard Sanchez and Norman J. McCormick

NEA No. 6292

NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

Infinite medium slowing down benchmarks

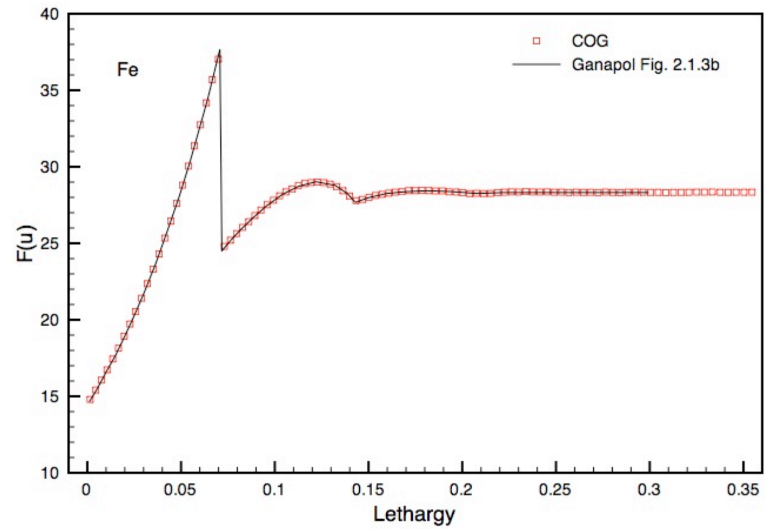
NEUTRON SLOWING DOWN AND THERMALIZATION

Benchmarks 2.1: Neutron slowing down in an infinite medium without spatial dependence and with constant cross sections.

Benchmark 2.1.2: Collision density vs. lethargy for neutrons slowing down in He.

Lethargy	Ganapol Table2.1.2	COG	sd(COG)	COG/ Ganapol	sd(COG)/ Ganapol
0.51083	2.08262	2.08290	0.00112	1.00013	0.00054
1.17057	2.26445	2.26580	0.00084	1.00060	0.00037
1.46840	2.34089	2.34070	0.00073	0.99992	0.00031
1.76624	2.36989	2.36990	0.00064	1.00000	0.00027
2.06407	2.33836	2.33810	0.00054	0.99989	0.00023
2.36191	2.35114	2.35130	0.00047	1.00007	0.00020
2.65974	2.35282	2.35300	0.00040	1.00008	0.00017
2.95758	2.35025	2.35040	0.00035	1.00006	0.00015
3.25541	2.35126	2.35150	0.00030	1.00010	0.00013
3.55325	2.35130	2.35240	0.00026	1.00047	0.00011
3.85108	2.35108	2.35270	0.00022	1.00069	0.00009

Benchmark 2.1.3b: The collision density vs. lethargy for Fe, showing the Placzek transient.



Slowing down benchmark results for 2.1.2, 2.1.3b, and 2.1.4 are excellent but ….

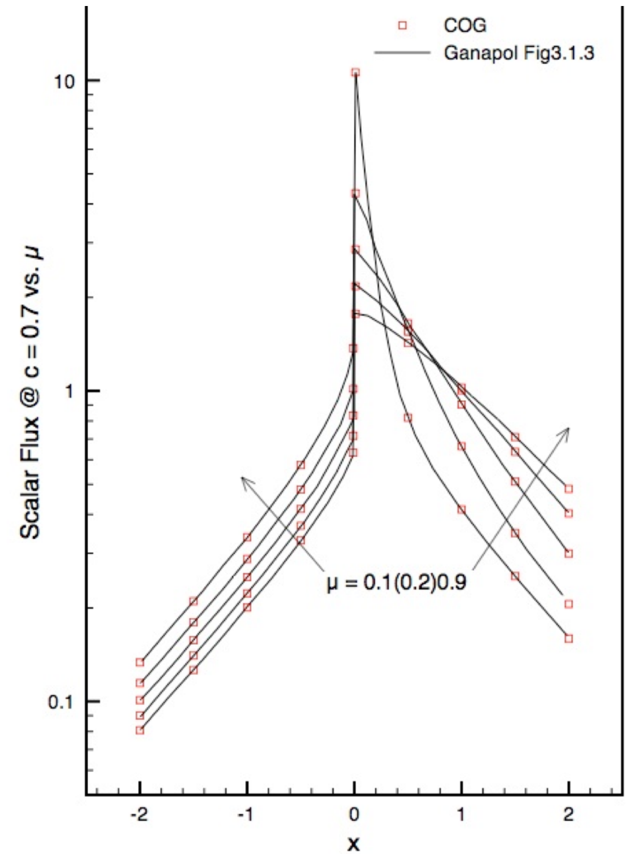
…. minor precision issues at high lethargies.

1-D transport benchmarks in planar geometry

Benchmarks 3.1: Neutron transport without energy loss in an isotropically scattering infinite medium including space dependence.

x	Ganapol Table 3.1.1	COG Scalar Flux	COG sd(Scalar Flux)	COG/Ganapol Scalar Flux	COG/Ganapol sd(Scalar Flux)
-5.00	1.02506E-01	1.0249E-01	3.2798E-05	0.99984	0.00032
-4.00	1.73596E-01	1.7356E-01	4.2525E-05	0.99979	0.00024
-3.00	2.94474E-01	2.9452E-01	5.5163E-05	1.00016	0.00019
-2.00	5.01677E-01	5.0171E-01	7.1268E-05	1.00007	0.00014
-1.00	8.66764E-01	8.6687E-01	9.2156E-05	1.00012	0.00011
-0.01	1.66724E+00	1.6676E+00	1.2792E-04	1.00022	0.00008
0.01	2.71018E+00	2.7098E+00	1.3686E-04	0.99986	0.00005
1.00	2.17754E+00	2.1777E+00	1.3443E-04	1.00007	0.00006
2.00	1.42338E+00	1.4234E+00	1.1401E-04	1.00001	0.00008
3.00	8.83953E-01	8.8397E-01	9.2654E-05	1.00002	0.00010
4.00	5.36683E-01	5.3669E-01	7.3533E-05	1.00001	0.00014
5.00	3.22109E-01	3.2211E-01	5.7566E-05	1.00000	0.00018

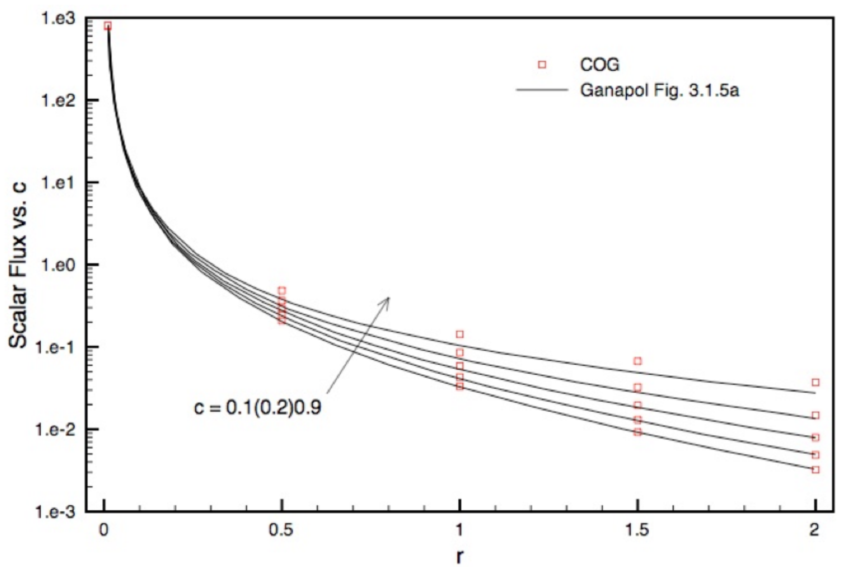
Benchmark 3.1.3: Infinite 1-D planar medium, scattering is zero energy loss and isotropic in the LAB frame, point source of neutrons at x = 0 beamed in the μ direction. Determine scalar flux @ c = 0.7 vs μ.



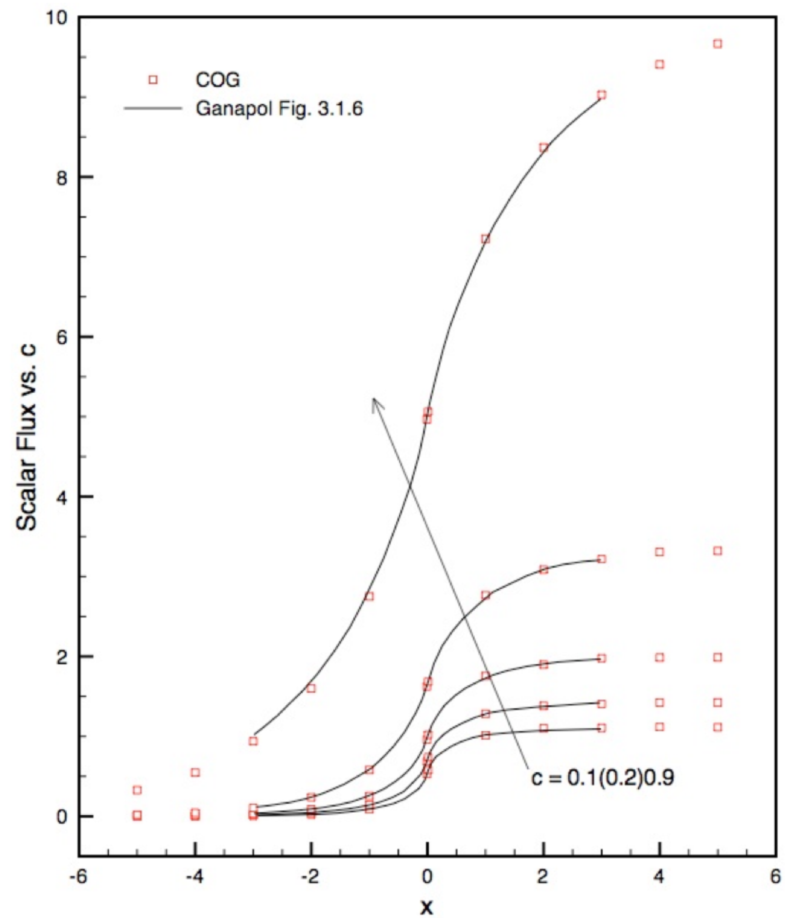
Infinite 1-D planar geometry transport benchmark results for 3.1, 3.1.2a, 3.1.2b, and 3.1.3 are excellent (as expected since 1-D cylindrical results reported in FY-2014 were also excellent).

1-D transport benchmarks in spherical geometry

Benchmark 3.1.5a: Infinite 1-D spherical medium, scattering is zero energy loss and isotropic in the LAB frame, isotropic point source of neutrons at x = 0. Determine scalar flux vs c.



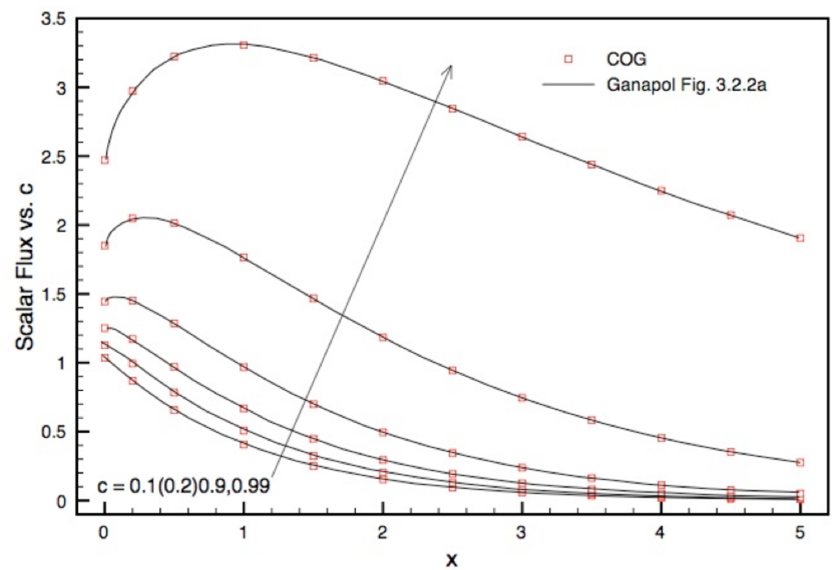
Benchmark 3.1.6: Infinite 1-D planar medium, scattering is zero energy loss and isotropic in the LAB frame, uniformly distributed source of neutrons in x > 0. Determine scalar flux vs c.



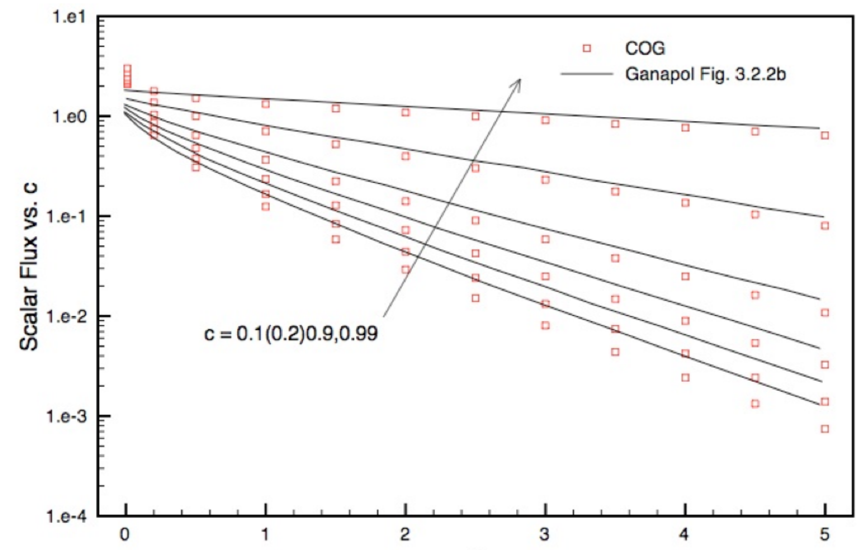
1-D spherical geometry transport benchmark results are either excellent (3.1.6) or have a possible issue with precision (3.1.5a, 3.1.5b).

Half-space "Milne" benchmarks

Benchmark 3.2.2a: Semi-infinite 1-D planar medium, scattering is zero energy loss and isotropic in the LAB frame, point source of neutrons at x = 0 beamed in x direction. Determine scalar flux vs c.



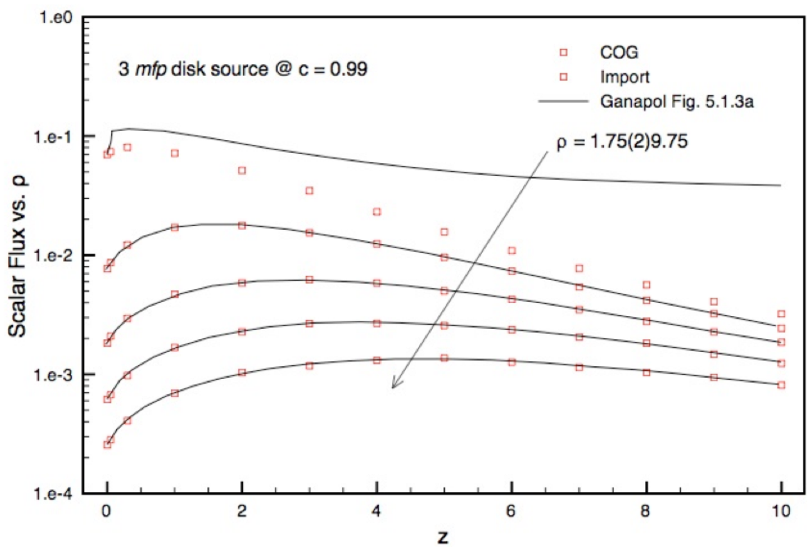
Benchmark 3.2.2b: Semi-infinite 1-D planar medium, scattering is zero energy loss and isotropic in the LAB frame, isotropic point source of neutrons at x = 0. Determine scalar flux vs c.



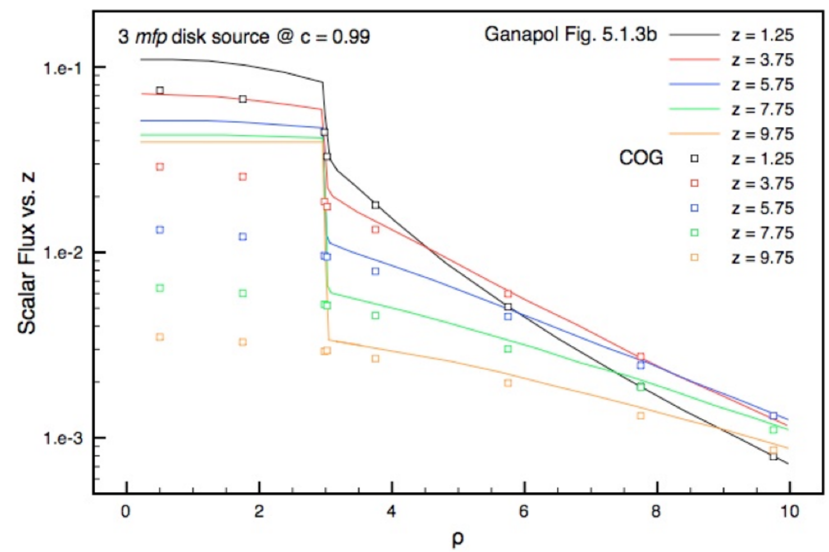
Semi-infinite transport benchmark results are either excellent (3.2.2a, 3.2.3, 3.3.1a, 3.3.1b, 3.3.2a, 3.3.2b) or in error (3.2.2b)

Multidimensional benchmarks

Benchmark 5.1.3a: Semi-infinite 2-D medium, scattering is zero energy loss and isotropic in the LAB frame, disk source of radius 3 *mfp* at x = 0 beamed in x direction for c = 0.99. Determine scalar flux vs ρ.



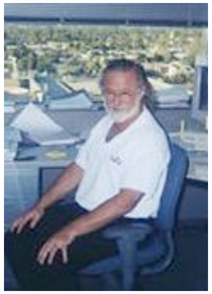
Benchmark 5.1.3b: Semi-infinite 2-D medium, scattering is zero energy loss and isotropic in the LAB frame, disk source of radius 3 *mfp* at x = 0 beamed in x direction for c = 0.99. Determine scalar flux vs z.



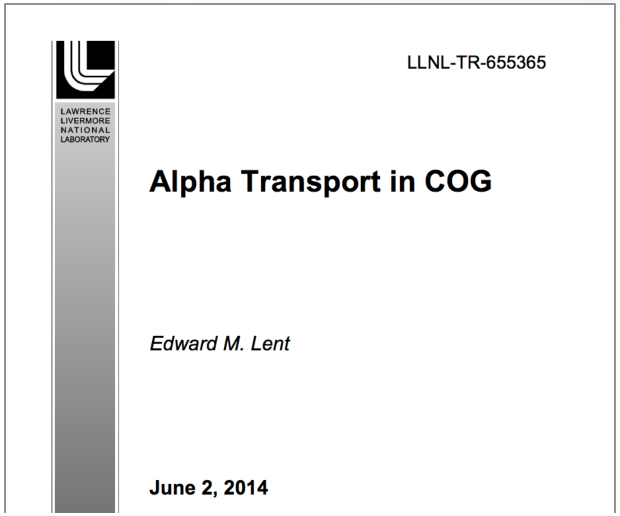
Multidimensional benchmark results are either excellent (5.1, 5.1.2, 5.1.4a, 5.1.4b) or have serious problems (5.1.3a, 5.1.3b)

Path forward

- Ed Lent is corresponding with the author to resolve noted discrepancies.
- These benchmarks are actually code-to-code inter-comparisons.
- Who's right?
- Anyone else study these benchmarks?
- If not, this is a possible topic for the NCSP Analytical Methods Working Group.



Alpha particle transport in COG



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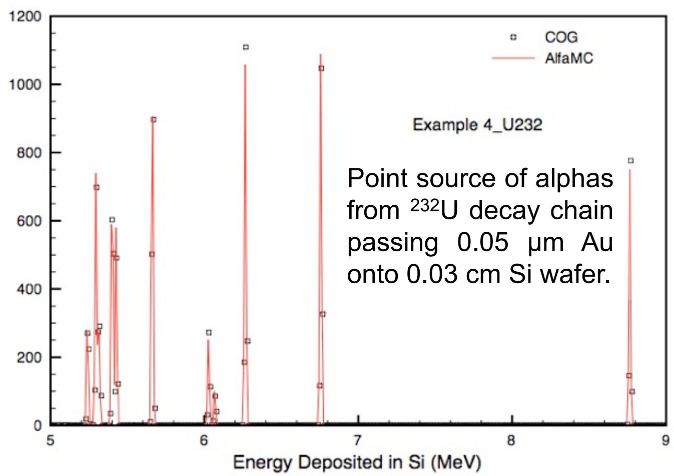
LLNL-TR-655365

Alpha Transport in COG

Edward M. Lent

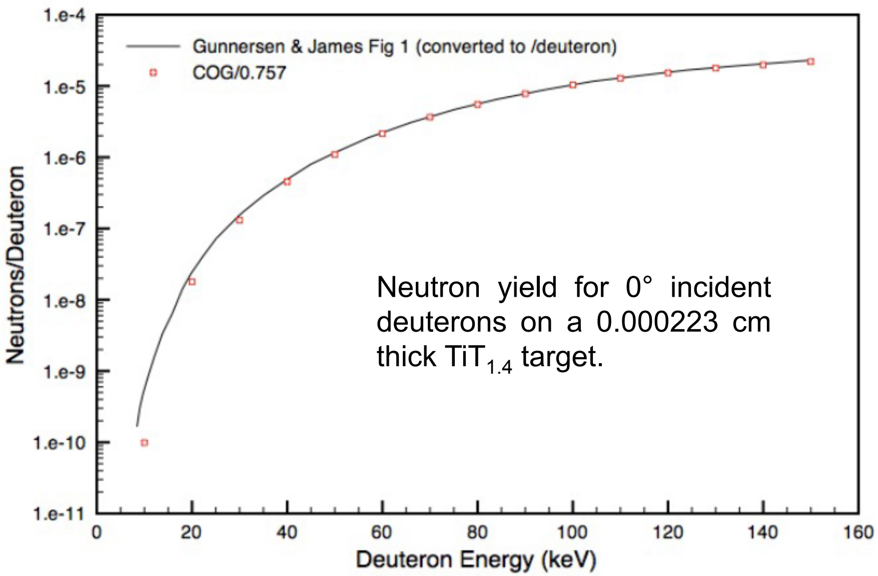
June 2, 2014



Thick Target (α,n) Neutron Yields, neutrons/10^6 α's															
		Calculation			Measured Values										
Target	E (MeV)	COG-JENDL	COG-TENDL	SOURCES	Ja83	We82	Ge80	Sm80	Ba79	Bu79	Ge75	An71	Go62	Ru56	Ro44
Be	2.0	1.000	0.732	0.873											
	2.5	1.000	1.050	0.948											
	3.0	1.000	1.598	1.060					0.844			0.866			
	3.5	1.000	2.071	0.997					0.828			0.932			
	4.0	1.000	2.087	0.979		0.979			0.852			0.904			
	4.5	1.000	1.784	1.034					0.875			0.915			
	5.0	1.000	1.556	0.993		0.991			0.863			0.620			
	5.3	1.000	1.429	0.978			1.015		0.876		0.890	0.959	1.17		1.11
	5.48	1.000	1.360	0.976			1.009	0.861						0.91	
	5.5	1.000	1.354	0.974					0.871		0.970				
	5.79	1.000	1.270	0.979			1.014								
	6.0	1.000	1.209	0.971		0.980		0.888							
	6.1	1.000	1.202	0.974			1.009							0.96	
	6.5	1.000	1.124	0.969				0.900							
C	3.0	1.000	1.400	1.450					1.200						
	3.5	1.000	1.472	1.417					1.111						
	4.0	1.000	2.289	1.500	1.026	1.132			1.105						
	4.5	1.000	2.864	1.477	1.045				1.068						
	5.0	1.000	2.867	1.350	1.017	1.083			1.050						
	5.3	1.000	2.356	1.310									1.3		1.03
	5.5	1.000	2.168	1.327	0.944				1.028						
	6.0	1.000	1.710	1.204		0.925			0.914						
	6.5	1.000	1.646	1.250					0.969						
N	6.5	1.000	2.718	3.103											
Al	3.5	1.000	1.938	0.500					0.750						
	4.0	1.000	1.559	1.039	1.250				1.112						
	4.5	1.000	1.387	0.957	1.006				0.927						
	5.0	1.000	1.210	0.867	0.802				0.816						
	5.3	1.000	1.231	0.873									1.34		1.13
	5.5	1.000	1.172	0.840	0.900				0.839						
	6.0	1.000	1.217	0.863					0.845						
	6.5	1.000	1.260	0.954					0.929						
Si	4.0	1.000	1.558	2.558	0.930	0.930									
	4.5	1.000	1.588	1.808	0.791				0.904						
	5.0	1.000	1.371	1.441	1.045	1.207			0.937						
	5.3	1.000	1.453	1.379									1.95		1.74
	5.5	1.000	1.388	1.220	0.944				0.952						
	6.0	1.000	1.162	1.054		0.947			0.879						
	6.5	1.000	1.167	2.683					0.885						

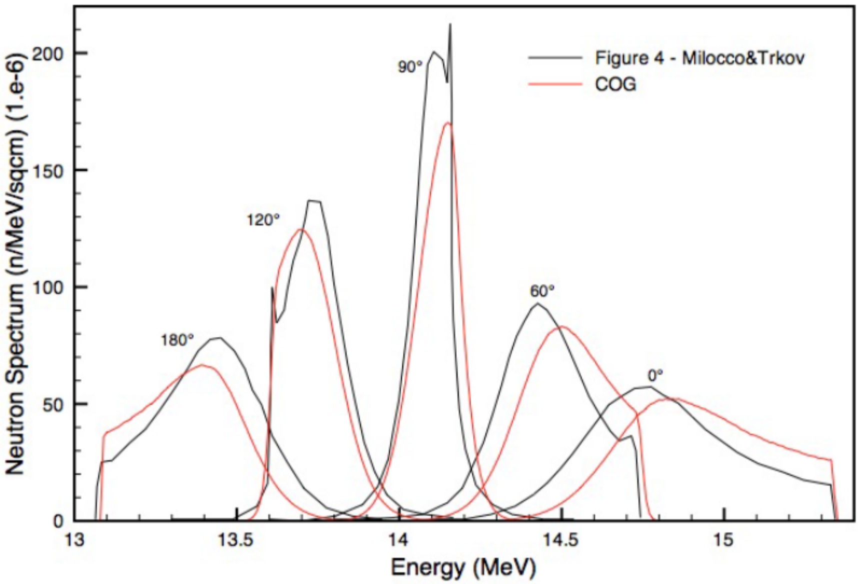
COG alpha transport is working well with the JENDL library which we have recommend for inclusion in ENDF/B. Need better experimental data and data for oxygen, fluorine, etc.

Deuteron transport in COG



Neutron yield for 0° incident deuterons on a 0.000223 cm thick $TiT_{1.4}$ target.

Comparison of calculated spectra from low voltage accelerated deuterons on titanium-tritium targets (see Hindawi, Publ. Corp., 2008, Article ID 340282, pp. 1-7).



Preliminary results look good. LLNL and Ohio integral pulsed sphere benchmarks are next.

ADVANCE

- Automated Data Verification and Assurance for Nuclear Calculations Enhancement
- LLNL provided BNL with:
  - COG11.1 code
  - COG “Libmaker” files (also at RSICC)
  - 503 COG ICSBEP benchmarks
- BNL is now enabled to test changes to cross section evaluations by automatically building new COG libraries (in ACE or ENDF formats) and running the available benchmarks.
- LLNL will provide additional benchmarks

The goal: upon every commit to the ENDF subversion repository, run all available checks on the uploaded files, automatically.

SQA

Table B-1, Software Quality Assurance Work Activities and Corresponding Documentation for Demonstrating Compliance

DOE O 414.1D SQA Work Activity	SQA Documents
1. Software Project Management and Quality Planning	– Software Project Management Plan (SPMP) and/or – Software Quality Assurance Plan (SQAP) ☒ – Software Safety Plan
2. Software Risk Management	– Various document types can be used to cover risk management ☑
3. Software Configuration Management	– Software Configuration Management Plan (SCMP) or related documents ☒
4. Procurement and Supplier Management	– Contractual documents or other procurement and use agreement documentation ☑
5. Software Requirements Identification and Management	– Software Requirements Specifications (SRS) or related document ☑
6. Software Design and Implementation	– Software Design Description (SDD), Model Description, Programmer's Reference Manual, or other related documents ☑
7. Software Safety	– SDD ☑ – Software Safety Analysis documentation ☑
8. Verification and Validation	– Verification and Validation Report ☑ – Test Case Description and Outcome Report; Other testing documents ☒
9. Problem Reporting and Corrective Action	– Software Error Notification and Corrective Action Report ☑
10. Training of Personnel in the Design, Development, Use and Evaluation of Safety Software	– User Instructions or User Manuals ☑ – Training Packages and User Qualification ☑
11. Model Validation and Evaluation	– Test results and evidence that code output was compared to experimental results or against equivalent output from an independent code and differences resolved ☑

New SQAP in development per ISQAP

New SCMP in development per ISQAP

Adding test cases with more detailed documentation.

Questions?

COG11.1 – New Features, Data, V&V

Rich Buck, Dave Heinrichs, Chuck Lee, Ed Lent

Lawrence Livermore National Laboratory, 7000 East Avenue, L-198, Livermore, CA, 94550, USA

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Paris - 2013

New Features

CritDetVR – Enables hybrid criticality/shielding calculations for variance reduction of detector scores with no bias in the keff calculation.
DFG – Simulates delayed gamma emission from the fission product decay.
NRF – Simulates nuclear resonance fluorescence reactions for nuclear photon absorption and emission.
RadSrc – Automatic photon source calculation for gamma emission from α-decay at a user-specified time (age).
COGLEX – Update includes dictionary entries for compounds with thermal scattering law.

New Data Libraries

NRF Library (Dr. Jim Hall, LLNL):
COGNRF
RadSrc Library (Dr. Ed Lent, LLNL):
COGRS
DFG Libraries (Dr. Ed Lent, LLNL):
DFG.ENDFB7R1
DFG.JEFF3.1.1
DFG.JENDL4
Neutron Libraries:
ENDFB7R1, PT.ENDFB7R1, T.ENDFB7R1
JEFF3.1.2, PT.JEFF3.1.2, T.JEFF3.1.2
JENDL4
Dosimetry Library:
IRDFF1.02
Supported Library Formats:
ENDL, ENDF, ACE
GND (in progress)
Many, many older data libraries continue to be supported (e.g., JEF2.2, ENDF/B-V).

MC-to-S_N

ARDRA – COG geometry package is included in LLNL's modern massively parallel S_N code with automatic meshing features.

V&V

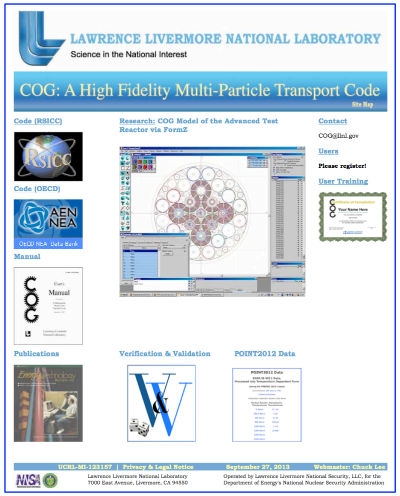
COG11BETA2 has been extensively tested using the following test suites:
- Regression tests (11 cases)
- ICSBEP criticality benchmarks (501 cases)
- NRF tests (3 cases)
- SINBAD shielding benchmarks (9 cases)
- SILENE Activation benchmarks (11 cases)
- PHOTONUCLEAR benchmarks (16)
- KOBAYASHI exact solutions (in progress)
- CRITCYL exact solutions (in progress)

Automation

LLNL is automating V&V code/data testing as described by M.-A. Descalle at ND2013. BNL is involved in a similar effort.

Website/Email

Please visit our website at http://cog.llnl.gov and contact us at COG@llnl.gov.



LLNL-POST-644394

COG11.1 – Practical Applications

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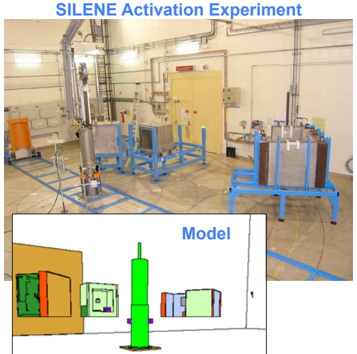
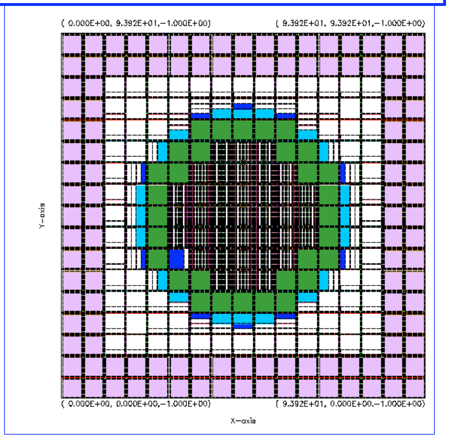
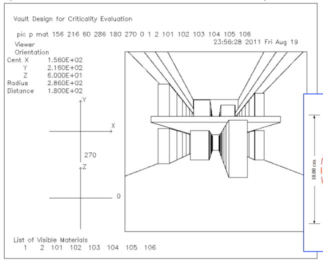
Paris - 2013

SILENE Activation Experiment

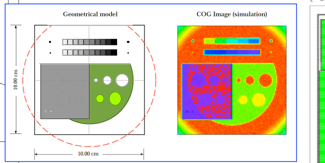




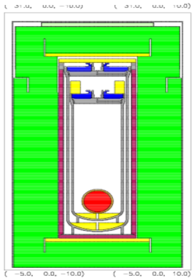
Detailed Model of ZPPR-21F
Reactor Physics



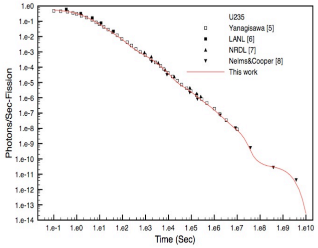
Storage Vault Model
Shielding & Criticality Safety



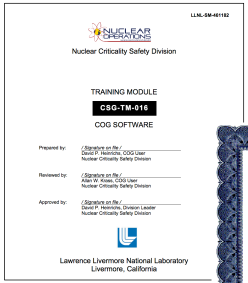
Neutron Radiography



9975 Shipping Container
Shielding & Criticality



Fission Product Decay Gammas
Dose Assessment



Practical User Training

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